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Quantitative prediction of cleavage fracture toughness of ferrite steel without adjustable parameters

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Abstract

This study presents a numerical model to quantitatively predict a cleavage fracture toughness of ferrite-cementite steel without any adjustable parameters. The model is constructed in framework of multiscale analysis. The macroscopic analysis is an elasto-plastic finite element analysis. A microscopic analysis is based on the Monte Carlo method considering microscopic fracture process of the three stages; Stage-I: formation of fracture origin by cementite cracking, Stage-II: propagation of the cementite crack into ferrite matrix and formation of a cleavage crack, and Stage-III: propagation of the cleavage crack across ferrite grain boundary. The predicted results of fracture toughness show good agreement with the experimental results including their scatter. Influences of microstructures on fracture toughness can be estimated by parameter studies. According to the results, the validation and the effectiveness of the proposed model are found out.

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Keywords: Cleavage fracture; Fracture toughness; Multiscale model; Fracture stress; Ferrite steel

1. Introduction

In order to prevent brittle fracture in steel structures, it is critically important to predict fracture toughness by clarification of crack initiation mechanism.

It is widely known that there is a strong correlation between a fracture toughness and microstructures of steel (Leslie 1981). For example, the finer grain makes the higher fracture toughness. The toughness depends on the size

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of brittle phase such as cementite. The reason has been, however, not clarified completely. Particularly, it has been difficult to quantitatively predict the fracture toughness based on only information of microstructures.

The cleavage fracture of steel is generally interpreted by the weakest-link mechanism differently from the yielding and the work hardening. Scatter is thus found in fracture toughness as its essential feature. This is a principal reason of the difficulty to quantify the influence of microstructures on fracture toughness. A formulation to evaluate the variation of fracture toughness was proposed by Beremin (1984) based on the weakest-link theory. We can find its effectiveness on quantitative evaluation of fracture toughness including its scatter. However, this model is not able to clarify the relationship between the fracture toughness and microstructures.

In the present paper, we propose a model to quantitatively predict the influence of microstructures on the fracture toughness of ferrite-cementite steels, based on the formulation of the cleavage fracture initiation process.

2. Formulation of Cleavage Fracture Initiation Process

2.1. Microscopic process of cleavage fracture initiation

We assume that the microscopic process of cleavage fracture initiation in ferrite-cementite steels is composed of three stages; (I) formation of fracture origin by cementite cracking, (II) propagation of the crack in cementite into the ferrite matrix and formation of a cleavage crack, and (III) propagation of the cleavage crack across ferrite grain boundary (see Fig. 1). It is assumed that a macroscopic brittle fracture occurs if a series of the fracture conditions of the above stages is satisfied. In the following section, the fracture conditions of respective stages are formulated.

2.2. Formulations of fracture conditions

- Formation of fracture origin by cementite cracking (Stage I)

It is known that a cracking of brittle phase such as cementite works as a trigger of cleavage fracture initiation.

We employ the probability of cementite cracking formulated in the author's recent study (Shibanuma *et al.*, 2013) as the fracture condition of Stage I. They formulated it as a function of cementite particle thickness and macroscopic stress and strain, based on an observation result and an estimation of internal stress of the cementite particle by FEA. A brief overview of the study is shown as follows.

It can be assumed that a cementite cracking occurs when the internal stress of cementite particle reaches to the fracture stress. Thus they formulated the probability of cementite cracking as a function of the size and the estimated value of the internal stress of cementite particle.

The estimation formula of internal stress σ_θ of the cementite particle from macroscopic stress and strain was developed as a function of the maximum principal stress $\sigma_{\max}$ and the equivalent plastic strain ε_{p}, based on the numerical results of FEA, as

$$\sigma_\theta = \sigma_{\mathrm{e}} + \sigma_{\mathrm{p}} = \frac{E_\theta}{E_\alpha}\sigma_{\max} + 0.179\,\sigma_{\mathrm{Y}}\left(\frac{\varepsilon_{\mathrm{p}}}{\varepsilon_{\mathrm{Y}}}\right)^{0.627} \tag{1}$$

where $\bar{\sigma}_{\mathrm{e}}$ and $\bar{\sigma}_{\mathrm{p}}$ are components depending on the elastic and plastic deformations, respectively.

Experiment was conducted by using steels with various sizes of microstructures were produced by laboratory scale vacuum melting and rolling. The ferrite grain sizes and cementite particle thickness was measured by combinations of a SEM observation, an EBSD analysis and an image analysis. Tensile tests using circumferential notched round bar specimens were then conducted. Distributions of cementite particle crack lengths were measured for various strain and stress conditions.

A nucleation of cementite cracking should be quantitated based on a stochastic framework because of its uncertainties such as distribution, shape, orientation and so on. The measured distributions of cementite particle thickness and crack length were approximated by introducing a distribution function considering upper limit. Eventually, the probability of nucleation of cementite cracking r_{c} was formulated as a function of cementite particle thickness t and the internal stress of the cementite particle σ_θ, as

$$r_{\mathrm{c}} = 0.0184\{\sigma_\theta - 1.03\}t^{2.47} \tag{2}$$

- Propagation of crack in cementite into ferrite matrix (Stage II)

We assume that a local fracture stress required for a propagation of a cementite crack into ferrite matrix. This condition can be formulated as

$$\sigma_{\mathrm{n}} \geq \sigma_{\mathrm{F}\theta\alpha} \tag{3}$$

σ_{n} is a maximum normal stress on the $\{100\}$-plane of the ferrite grain because it is known that a cleavage fracture surface in a BCC polycrystal including ferrite-cementite steel are generally formed on a $\{100\}$-plane. σ_{n} is calculated as

$$\sigma_{\mathrm{n}} = \max_{m=1,2,3} (\mathbf{n}_m)^T \cdot \boldsymbol{\sigma} \cdot \mathbf{n}_m \tag{4}$$

where $\mathbf{n}_m$ is a normal vector of the m-th $\{100\}$-plane and $\boldsymbol{\sigma}$ is a applied stress tensor. $\sigma_{\mathrm{F}\theta\alpha}$ in Eq (3) is the fracture stress originally proposed by Petch (1986) as

$$\sigma_{\mathrm{F}\theta\alpha} = \begin{cases} \dfrac{4E\gamma_{\theta\alpha}}{\left(1+\dfrac{1}{\sqrt{2}}\right)(1-\nu^2)k_y\sqrt{s}} & (t_\theta < c_c) \\ \sqrt{\dfrac{4E\gamma_{\theta\alpha}}{\pi(1-\nu^2)t_\theta} - \dfrac{k_y^2 s}{8\pi^2 t_\theta^2} - \dfrac{k_y\sqrt{s}}{2\sqrt{2}\pi t_\theta}} & (t_\theta \geq c_c) \end{cases} \tag{5}$$

where ν is a Poisson's ratio. The definition of $\sigma_{\mathrm{F}\theta\alpha}$ is slightly modified from the original one by replacing a ferrite grain diameter with a length of the dislocation line s. k_y is a locking parameter in the Hall-Petch law and is assumed to equal 20.7 MPa mm$^{1/2}$ based on our preliminary test. $\gamma_{\theta\alpha}$ is effective surface energy and is given as 10 J/m^2. c_c is critical cementite particle thickness defined as

$$c_c = \frac{\left(1+\dfrac{1}{\sqrt{2}}\right)(1-\nu^2)k_y^2 s}{8\pi E\gamma_{\theta\alpha}} \tag{6}$$

$\sigma_{F\theta\alpha}$ is derived from a comparison of the sum of energy release rate of the crack and piled-up dislocation energy with the effective surface energy.

- Propagation of cleavage crack across ferrite grain boundary (Stage III)

We also assume a local fracture criterion for Stage III, as

$$\sigma_{\mathrm{n}} \geq \sigma_{\mathrm{F}\alpha\alpha} \tag{7}$$

where $\sigma_{\mathrm{F}\alpha\alpha}$ is local fracture stress for Stage III formulated based on the Griffith theory, as

$$\sigma_{\mathrm{F}\alpha\alpha} = \sqrt{\frac{\pi E\gamma_{\alpha\alpha}}{(1-\nu^2)D}} \tag{8}$$

where D is a diameter of cleaved surface formed in Stage II and $\gamma_{\alpha\alpha}$ is an effective surface energy for a cleavage crack in a ferrite grain to propagate across grain boundary. It is assumed that $\gamma_{\alpha\alpha}$ depends on temperature based on the experimental results by San Martin and Rodriguez-Ibabe (1999) because plastic deformation below cleavage

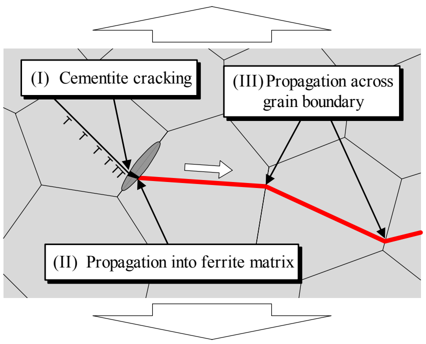


Fig. 1. Cleavage fracture initiation process

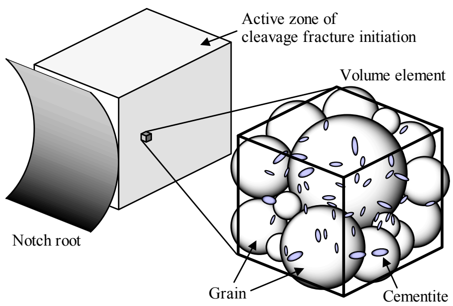


Fig. 2. Model for microscopic analysis

fracture surface changes with temperature.

3. Development of Prediction Model

A multiscale model to predict the cleavage fracture toughness of ferrite-cementite steels is developed. The macroscopic analysis is an elasto-plastic FEA. The microscopic analysis is based on the above fracture conditions of three stages and the Monte Carlo method. A procedure of the modeling is described as follows.

(i) A domain where the cleavage fracture initiation is possible to occur is defined as an active zone.
(ii) The active zone is divided by cubic volume elements of the same size. A schematic view of the active zone and volume element is shown in Fig. 3.
(iii) Ferrite grains are assigned at random in each volume element based on ferrite grain size distribution until sum of the volumes of assigned grains reaches the elemental volume. Crystallographic orientation of each grain is determined at random at the same time.
(iv) Cementite particles are assigned in each volume element based on cementite particle thickness (minor axis) distribution. The shape of the cementite is approximated as a prolate spheroid.
(v) Stress tensor and equivalent plastic strain at each volume element are evaluated by macroscopic elasto-plastic FEA using true stress-strain curve.
(vi) In a calculation, step time increments are defined. And then, the cleavage fracture initiation process based on the three stages is evaluated in each volume element for each time step as following (viii) ~ ().
(vii) For Stage I, cracked cementite particle distribution is evaluated based on Eqs. (1) and (2) by using the distribution of cementite particle thickness in the volume element.
(viii) For Stage II, first, two ferrite grains (Grain A and Grain B) next to the respective cracked cementite obtained in (vii) are selected at random. Grain A and Grain B are used for the evaluation of σ_{n} in Eq. (4) and $\sigma_{\mathrm{F}\theta\alpha}$ in Eq. (5), respectively. Assuming the location of the each cementite particle on the boundary of Grain B, the length of dislocation line s is determined. Then, the fracture condition of Stage II is evaluated based on Eq. (3) for all the combinations of the ferrite grains and the cracked cementite particles. If the fracture condition is satisfied, a cleavage crack forms in Grain A and the cleaved grain is excluded in following time steps.
(ix) In the case that Stage II is satisfied, Stage III is then evaluated based on Eq. (7). $\sigma_{\mathrm{F}\alpha\alpha}$ in Eq. (8) is calculated by using the size and direction of the cleavage crack formed in Grain A.
(x) Cleavage fracture is assumed to be initiated at the time when the fracture condition of Stage III is satisfied in any one of the volume elements. That is a “weakest link” assumption in this model.
(xi) If the fracture is not initiated, the procedures of (vii) ~ (x) are carried out for the next time step.

4. Prediction of Fracture Toughness

4.1. Experiment

Three point bending test using notched specimens as shown in Fig. 4 were used for validation of the proposed model. Quasi-CTOD is introduced as a parameter to evaluate the fracture toughness by simply applying the CTOD estimation formula of BS 7448 (1991), as

$$\delta = \frac{K^2(1-\nu^2)}{2\sigma_{\mathrm{Y}}E} + \frac{r_{\mathrm{p}}(W-a)V_{\mathrm{p}}}{r_{\mathrm{p}}(W-a)+a} \tag{9}$$

where K is a stress intensity factor, r_{p} is the rotation factor ($= 0.4$), W is the width of the specimen ($= 20\mathrm{mm}$), a is the notch depth ($= 7\mathrm{mm}$) and V_{p} is plastic component of the notch opening displacement. It is noted that the quasi-CTOD does not represent physical crack tip opening displacement but just represents intensity of deformation at the notch root.

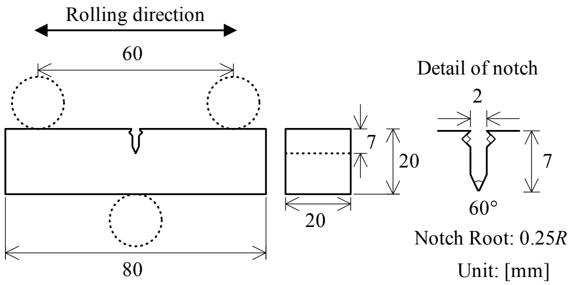


Fig. 3. Configuration of notched three point bend specimen

Table 1. Carbon concentration and representative ferrite grain size and cementite particle thickness of each steel

Symbol		10LL	10LS	5SL
Carbon concentration [mass%]		0.1	0.1	0.05
Ferrite grain diameter [× 10^{-3} mm]	Average	57	58	27
	Max	218	229	67
Cementite thickness [× 10^{-3} mm]	99%max	0.83	0.24	0.66
	Max	1.87	0.66	1.15

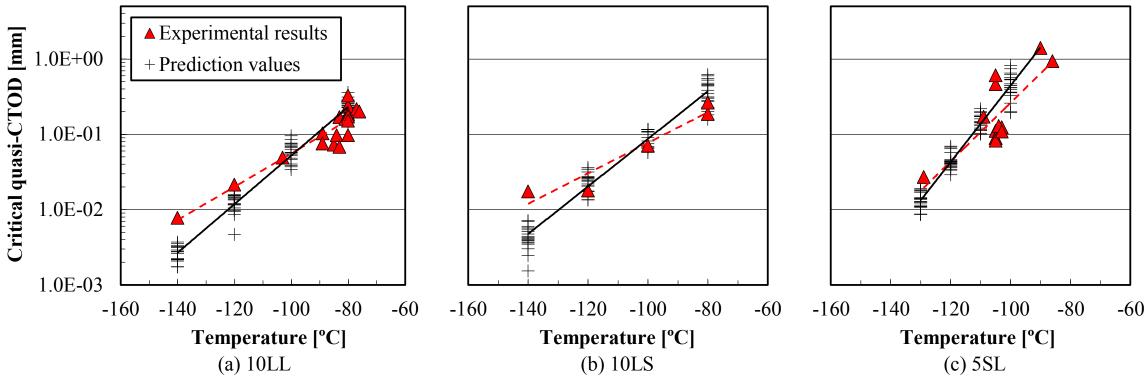


Fig. 4. Comparison of prediction values with experimental results

Three types of steel, 10LL, 10LS and 5SL, were employed. The carbon concentration and representative ferrite grain size and cementite particle thickness of the respective steel are shown in Table 1.

4.2. Model conditions

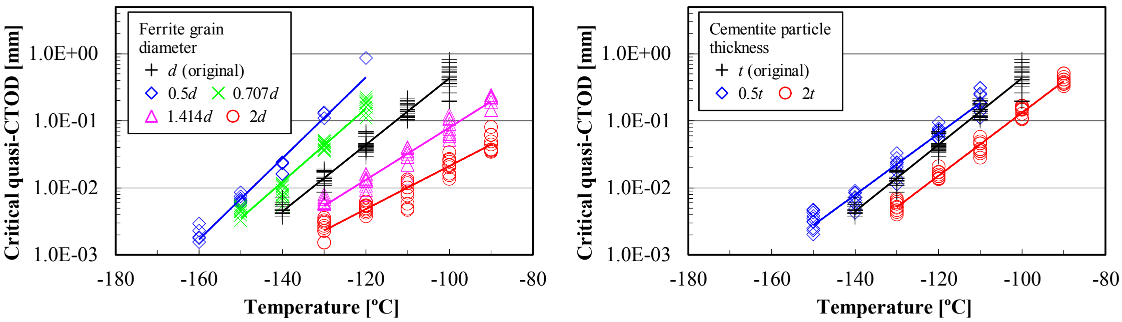
In the procedure (i), the active zone is defined as a rectangular parallelepiped whose side lengths are 1.6 mm, 1 mm and 20.0 mm in respective directions of the width, the axis and the thickness of the specimen, based on the preliminary observation of the fracture initiation points. The size of each volume element in the procedure (ii) is also defined as a rectangular parallelepiped. The side lengths are 0.2 mm, 0.167 mm and 0.2 mm in the respective directions. The number of the volume elements is 4,800 in the active zone as a result. In the procedures (iii) and (iv), The ferrite grains and the cementite particles are assigned at random in each volume element based on their observation results. A quarter-symmetry finite element model is used to obtain stress and strain distributions in the active zone in the procedure (v).

4.3. Validation of Proposed Model

Comparisons of the experimental results and the prediction values of the critical quasi-CTOD are shown in Fig. 4. The predicted values show good agreements with the experimental results in all the steels though the proposed model does not use any adjustable parameters. The scatter of toughness can be reproduced in the prediction. This scatter is derived from the stochastic nature of the developed model, i.e., the distributions of ferrite grains and cementite particle introduced by the Monte Carlo method.

4.4. Quantitative prediction of influence of microstructures on fracture toughness

In order to quantify the influence of microstructures on fracture toughness, a parameters study is conducted. The distributions of ferrite grain diameter and cementite particle thickness of 5SL are employed as the standard.



(a) Influence of ferrite grain size (b) Influence of cementite particle size

Fig. 5. Influence of ferrite grain and cementite particle sizes on fracture toughness

The results are shown in Fig. 5. We can find the quantitative effect of the refinement of ferrite grain and cementite particle. It can be estimated that the finer grain does not only make the higher fracture toughness but also the larger gradient of the toughness. It can also be estimated that refinement of cementite particle has smaller influence than that of ferrite grain. Based on the aforementioned results, the validation and the effectiveness of the proposed model are found out.

5. Conclusion

A model to quantitatively predict cleavage fracture toughness in ferrite-cementite steel without any adjustable parameters was developed. The model is based on the multiscale framework. The macroscopic analysis is FEA. The microscopic analysis is based on the Monte Carlo method considering microscopic fracture process of three stages.

The developed model was validated by three point bend testing of notched specimens using steels with various ferrite and cementite sizes. The numerical predicted values of fracture toughness show good agreement with the experimental results for all cases including the scatter of toughness. It is therefore concluded that the proposed model showed its effectiveness to predict the fracture toughness of ferrite-cementite steels.

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